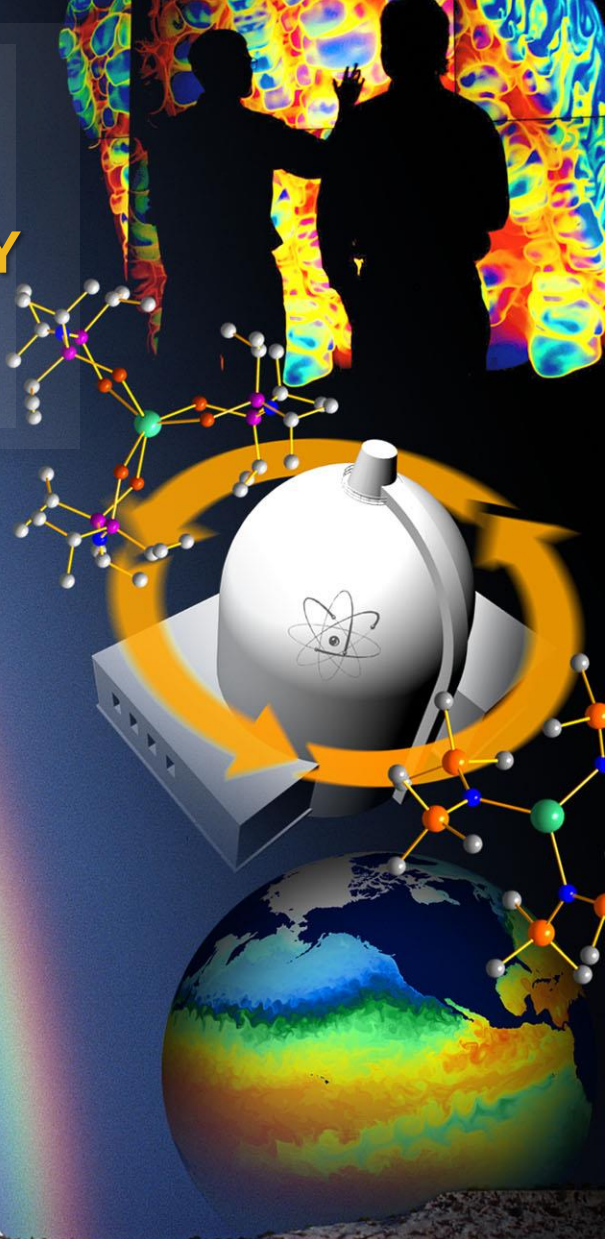
LOS ALAMOS
A NATIONAL SECURITY SCIENTIFIC LABORATORY FOR THE 21ST CENTURY

Alan Bishop

March 2015



The nation's investment in Los Alamos has fostered scientific capabilities for national security missions

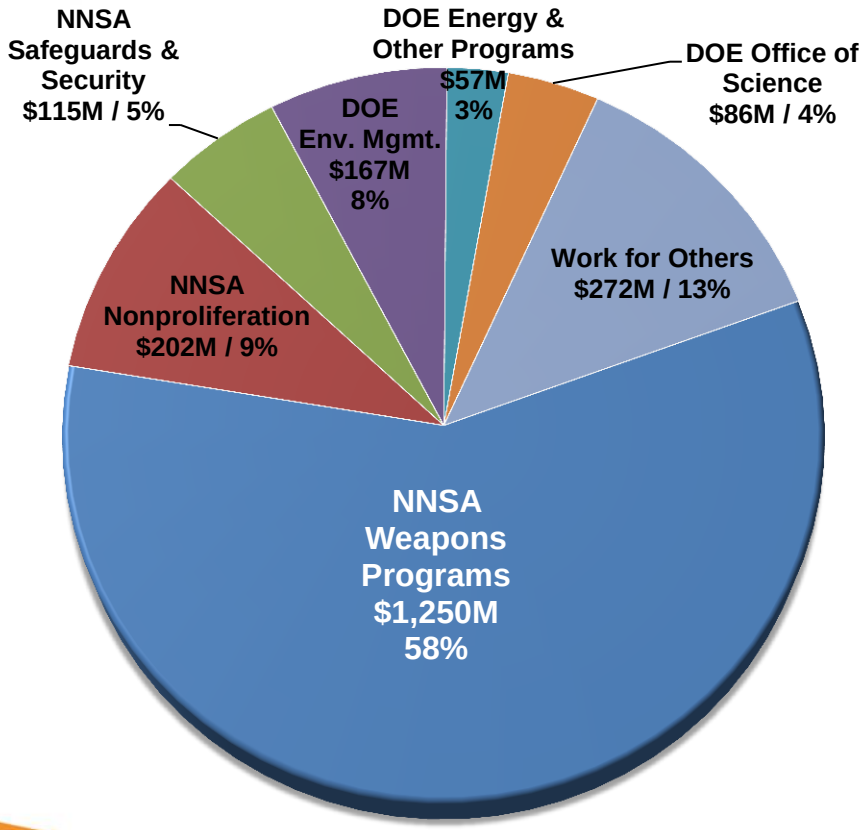
As a Premier National Security Scientific Laboratory, Los Alamos tackles:

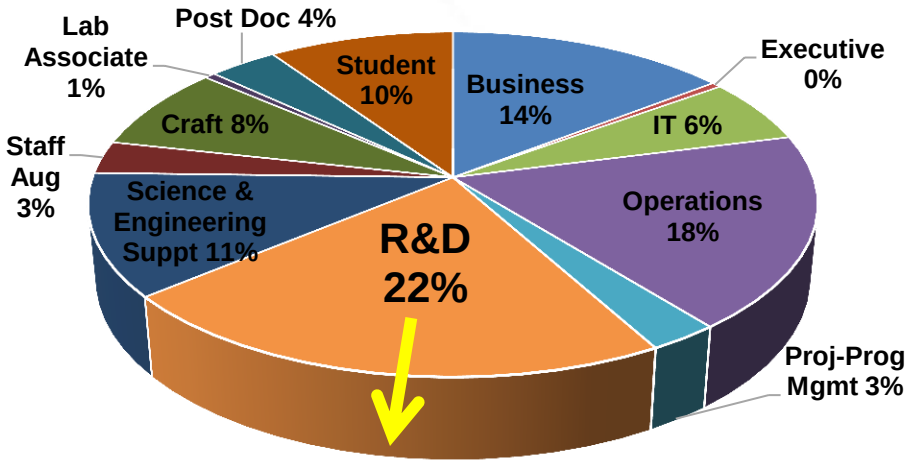
- Multidisciplinary science, technology, and engineering challenges
- Problems demanding unique experimental and computational facilities
- Highly complex national security issues requiring fundamental breakthroughs

Applying multidisciplinary capability
is inherent in our broad program and workforce base

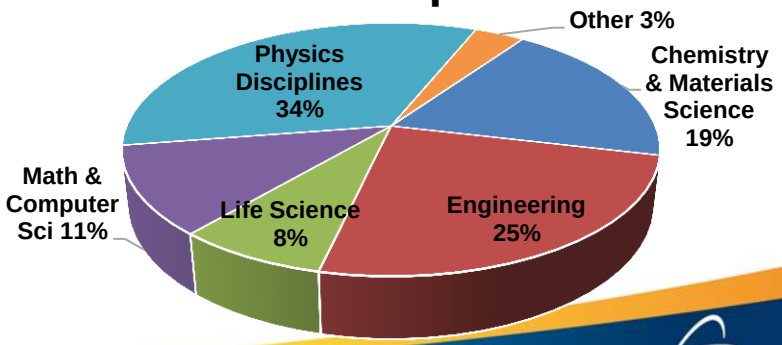
FY15 est. Budget Authority: $2.15B

Approx. 10,000 National Security specialists collaborate on a 36-sq.-mile site in a wide variety of technical disciplines



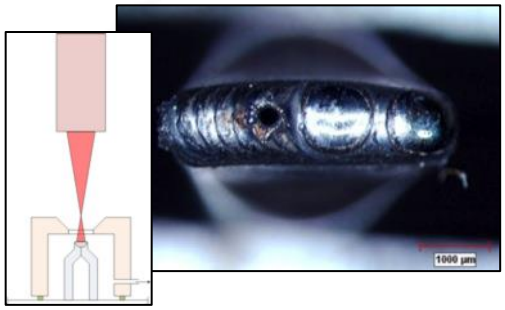


R&D Disciplines

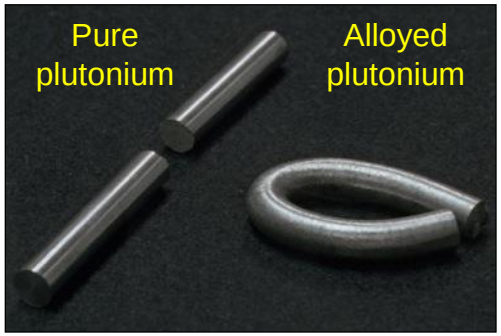


As a National Security Scientific Laboratory, Los Alamos maintains broad and deep STE capabilities for multi-program leverage

Stockpile Stewardship



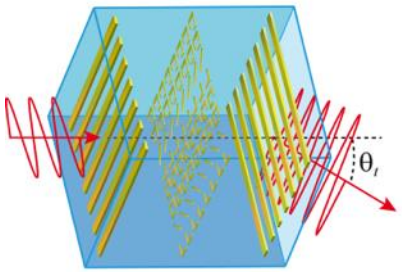
Weapons Assessment
Nondestructive laser gas sampling



Plutonium Science
Metallurgy

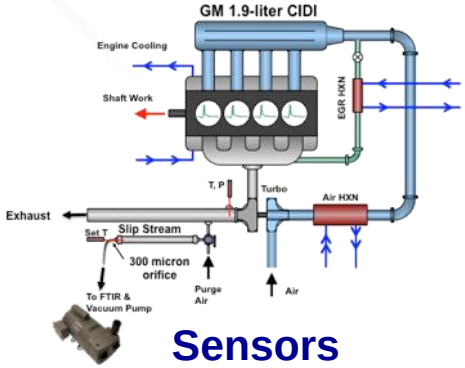
Global Security

Research Reactor Conversion
High flux isotope reactor



Terahertz Metamaterials
Electromagnetic wave polarization and propagation

Energy Security



Sensors
Nitrogen oxide and ammonia sensors

Materials
Energy generation & transmission

A robust ecosystem for scientific vitality and mission impact

Reciprocal pipelines of People, Ideas, Partnerships

Fundamental Science Program

LDRD

Aligns innovative capability with strategic program directions

Community Involvement

- Conferences
- Professional Service

International User Facilities

Center for Integrated Nanotechnologies

National High Magnetic Field Laboratory

Los Alamos Neutron Science Center

SCIENTIFIC VITALITY

National Security Education Center

- Institutes
- Students
- Postdocs

Strategic Partnerships

- Agencies
- Universities
- Labs
- Industry

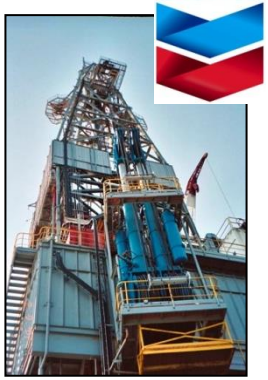
Mission Facilities

Los Alamos leverages its intellectual assets through strategic 'win-win' partnerships

Technology Transfer

"Results from our reliability technology partnership with Los Alamos will reduce P&G costs by $1.5B annually."

–Mark Peterson, Procter & Gamble



Labs & Universities

ExMatEx

U.S. DEPARTMENT OF ENERGY

International Partnerships

Japanese Ministry of Technology (NEDO) with Los Alamos County

New Mexico Consortium

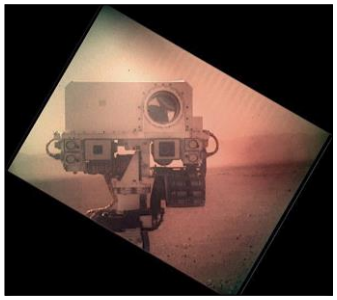
PRObe Supercomputing Center ribbon-cutting

NSF

Our partnerships are strategic and diverse, e.g.

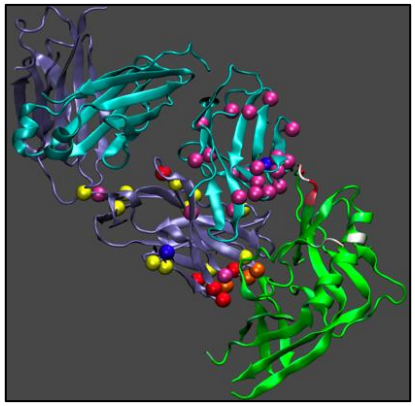
Science of sensors extend to multiple applications

Remote sensing and detection have applications everywhere — from Mars Rover to non-proliferation, space, defense, and intelligence.




Global partners advance AIDS research

Los Alamos developed the “mosaic vaccine” concept: a predictive framework to identify the most active epitopes in the immune system response and apply to a vaccine strategy.



We provide databases, theory, simulation, and high-performance computing design tools to the Global HIV Vaccine Enterprise and the CHAVI Consortium.

Los Alamos Science, Technology & Engineering Capability Pillars

Build cross-disciplinary teaming experience and confidence for current and future missions

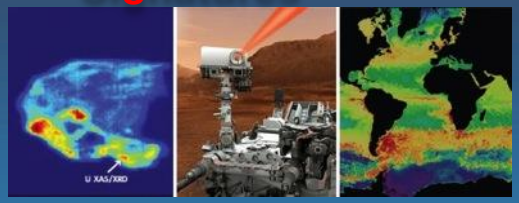
SCIENTIFIC EXCELLENCE FOR NATIONAL SECURITY

LANL MISSIONS

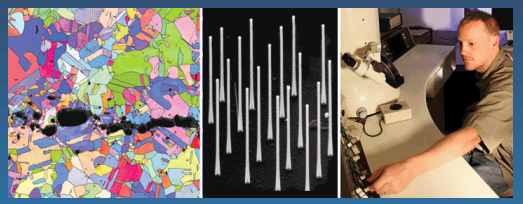
- Nuclear Deterrence
- Global Security
- Energy & Emerging Threats

Integrating Assets for Program Execution

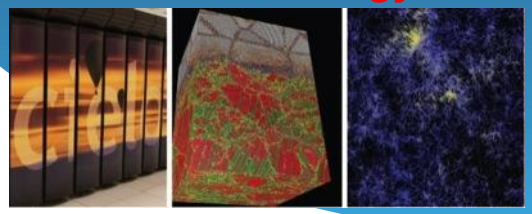
Science of Signatures



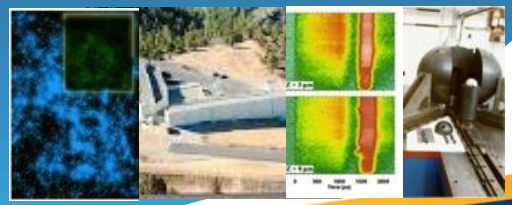
Materials for the Future



Information, Science, and Technology

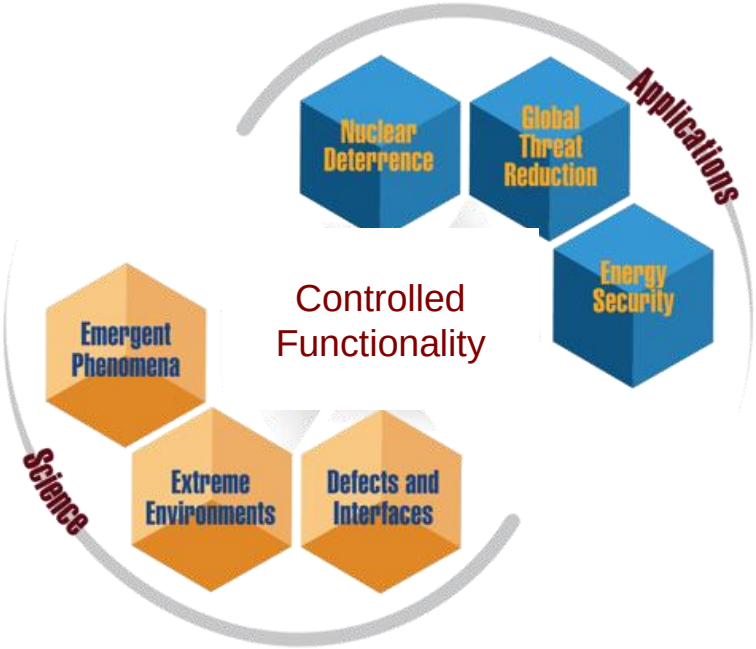


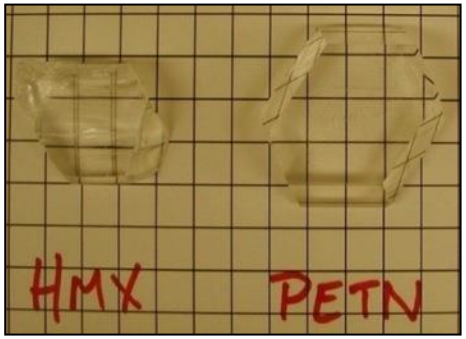
Nuclear and Particle Futures

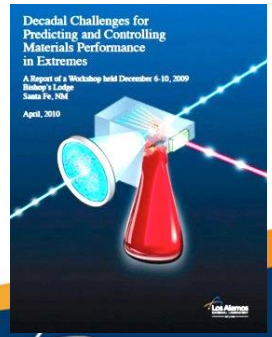


Los Alamos Materials Strategy —
The result of a many-decade iteration of STE & Missions

The Materials Capability Pillar advances our vision to develop materials with "controlled functionality" to provide solutions enabling Los Alamos' missions







Thrusts define the Areas of Leadership for the Materials Pillar

Actinide and Correlated Electron Materials

- Understanding and controlling emergent electronic states
- Actinide materials science center of excellence
- Predicting and controlling plutonium aging and lifetime

Integrated Nanomaterials

- Center for Nanophotonics
- Center for Strategic Nanomaterials

Materials in Radiation Extremes

- Advanced nuclear fuels nuclear waste materials
- Advanced radiation temperature tolerant structural materials

Energetic Materials

- Prediction and control of explosives safety, initiation, and performance
- Invent and utilize revolutionary diagnostics

Materials Dynamics

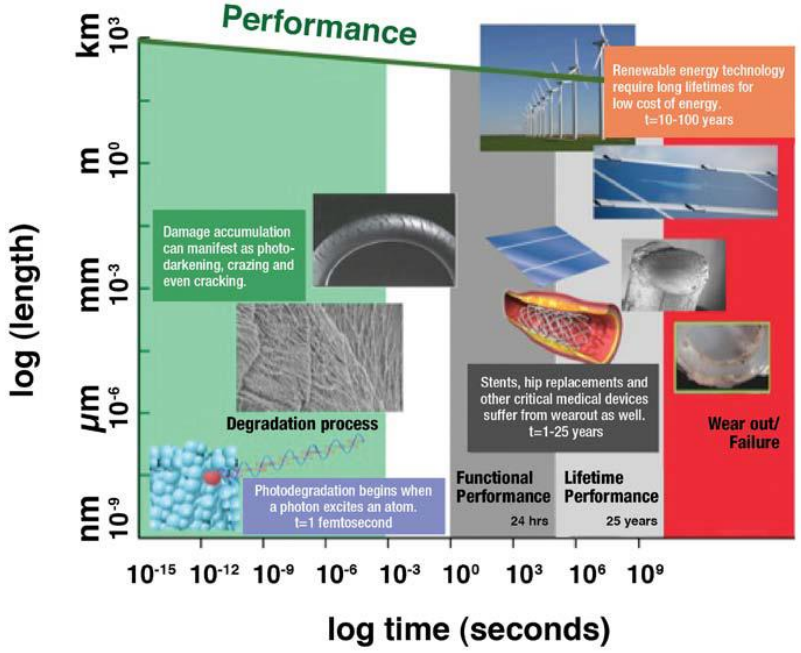
- Linking material microstructure to macroscopic behavior under dynamics deformation conditions
- Prediction and control of dynamic processes
- Next generation diagnostics, dynamic drivers, and predictive models

Complex Functional Materials

- Bio-inspired materials
- Materials for energy conversion, storage, and transmission

We are not alone in our interest in "microstructure to performance" —
Los Alamos is involved broadly with the community

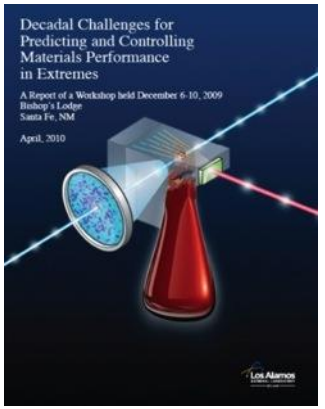
The "mesoscale" challenge is to observe the dynamic evolution of polycrystalline materials at the granular and sub-granular level



Sub-μm resolution 100's – 1000's μm samples; Sub-ns resolution, ~30 frames in1 μs duration

meso2012.com

Materials Genome



science.energy.gov

Whitehouse.gov

Advanced (including Additive) Manufacturing:

Prediction and control of manufacturing processes

— bringing "Science," "Engineering" & "Manufacturing" closer —

Lightweight materials

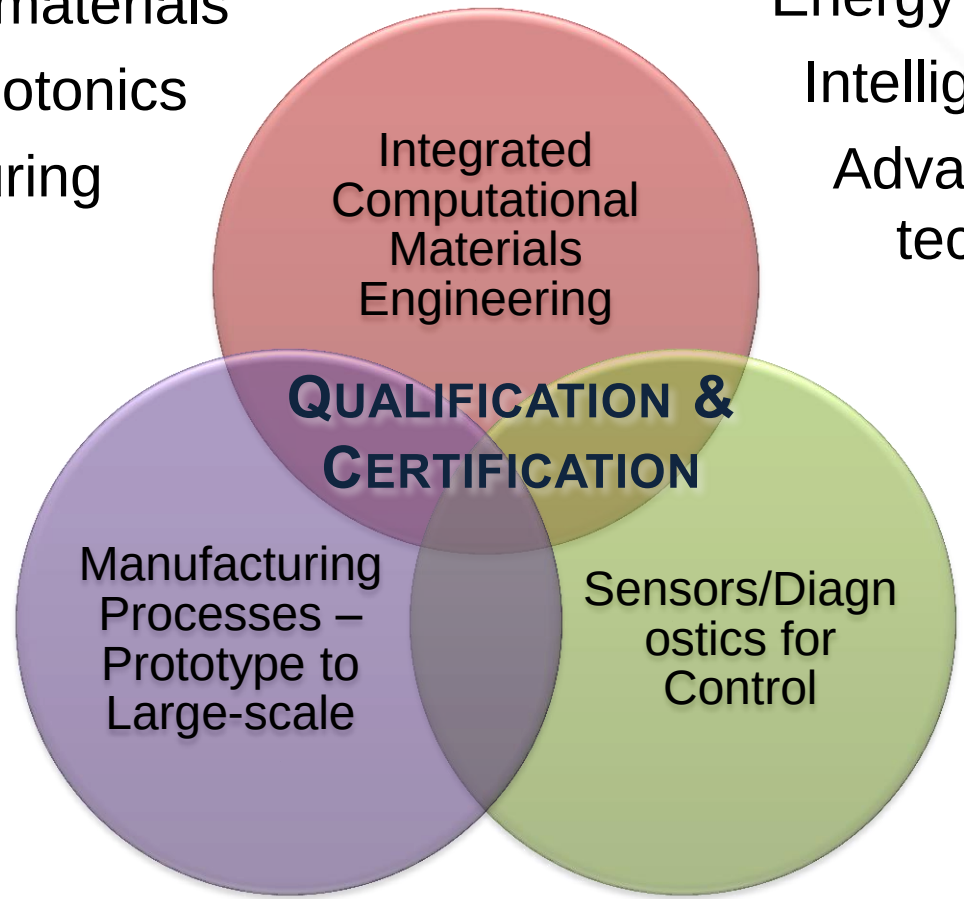
Advanced photonics

Biomanufacturing

Energy futures/extraction

Intelligent manufacturing

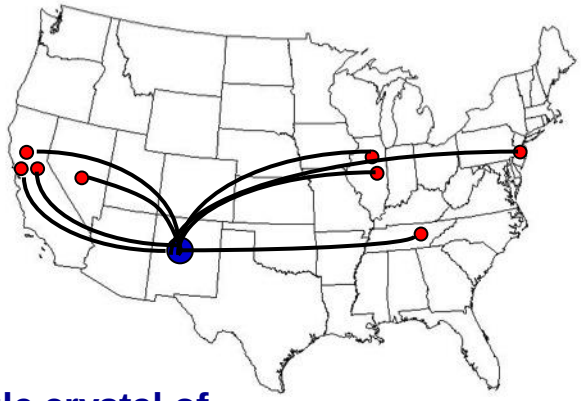
Advanced fabrication technologies



Los Alamos' Plutonium S&R Strategy supports National Plutonium Stewardship

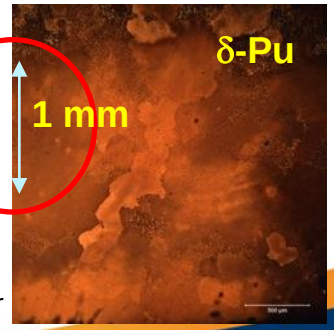
Many experiments at national user facilities enabled by special isotopes and radiological facilities

- n-scattering on $^{242}PuCoGa_5$ single crystals and δ-^{242}Pu at LANSCE, NIST, and SNS (30 g Pu)
- Produced ~1 mm single crystal grains of δ-Pu
- Determination of multi-configurational ground states in α & δ-Pu
- X-ray Emission (XES) under pressure shows 6d/5f hybridization
- Observed Fermi surface pocket in $PuIn_3$ single crystals
- Discovery of Superconductivity in $PuCoIn_5$ and $PuRhIn_5$
- Full elastic tensor of $^{242}PuCoGa_5$ via Resonant Ultrasound Spectroscopy (RUS)



single crystal of $^{242}PuCoGa_5$

single crystal of δ-Pu



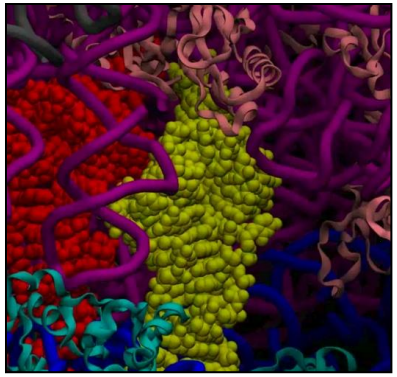
Eric Bauer

Los Alamos has a distinguished 70-year supercomputing history

Fidelity at scale: Data-informed, "adaptive-physics," multi-scale simulation tools essential for "complex systems"

Examples:

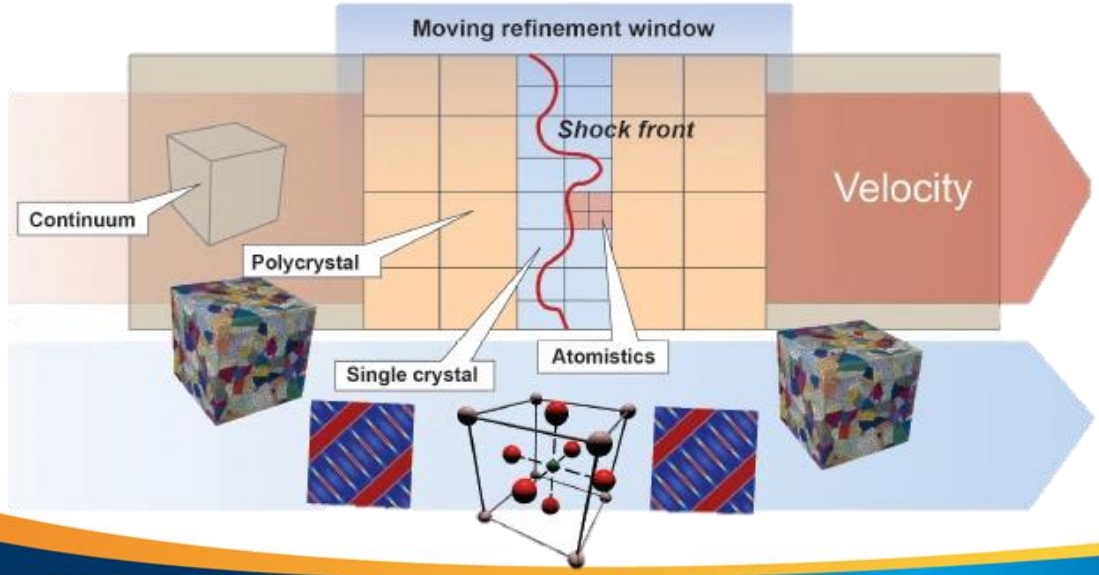
BIOLOGICAL MACHINES



ENERGY-CLIMATE IMPACTS

Climate Models: Atmosphere, Ocean, Land, Ice

MATERIALS



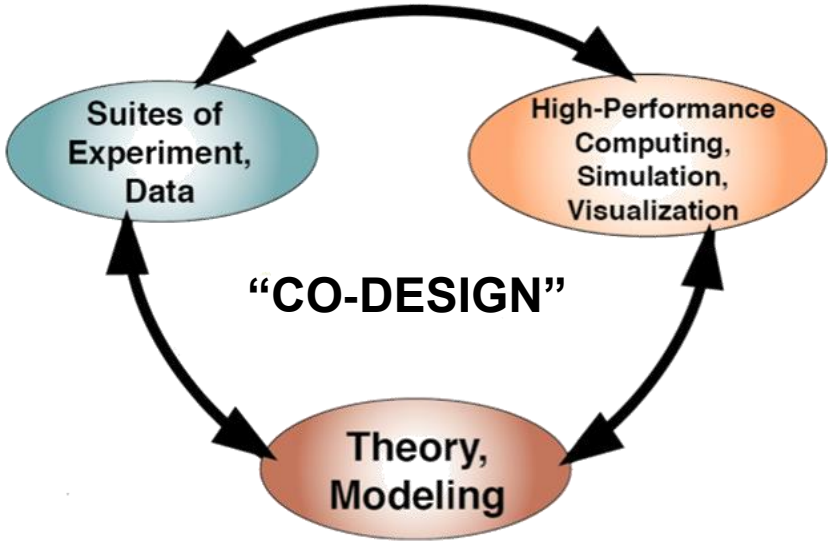
The future of Materials Science:
Control science via integration

Control Science

- Accelerated materials discovery and design

Integration

- Key to prediction of material properties
- Theory and models that take function to structure
- Synthetic control of defects and interfaces



- Characterization of the evolution of defects and interfaces in multiple extremes to provide feedback

National Security and Prosperity in the "Century of Complexity"

Building on Los Alamos' 70-year heritage

Mission Complexity

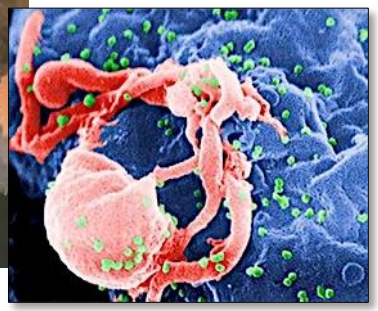
Nuclear Deterrence

Climate Change

Global Resources

Contested/ Congested Space

Environment



Health

ST&E Complexity

Science of prediction & **Uncertainty quantification**

Methodologies for

Complex Natural & Engineered Systems

- Strategic deterrence
- Complex materials, Advanced manufacturing
- Energy, climate, environment
- Biological systems
- Space
- Cyber

Data ➡ Knowledge ➡ Control;

Quantitative tools for decision-makers/risk assessment

The Pivot to Asia

Allies Seeking Assurances of US Guarantees

Nuclear Proliferation

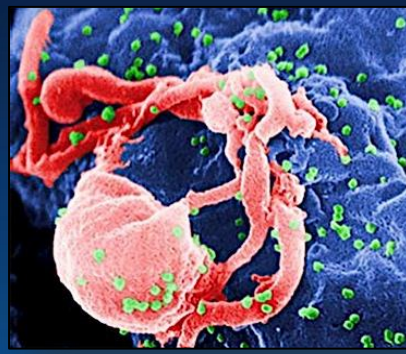
Ukraine – Russian Incursion

Climate Change

Global geopolitical backdrop is increasingly fluid, complex, and dangerous

Our STE needs to be ready

Global Pandemics



Contested Space

Terrorism & the Increasing Reach of Technology

Instability

National Security challenges & technologies are accelerating: How Los Alamos works is needed more than ever for national security … and prosperity

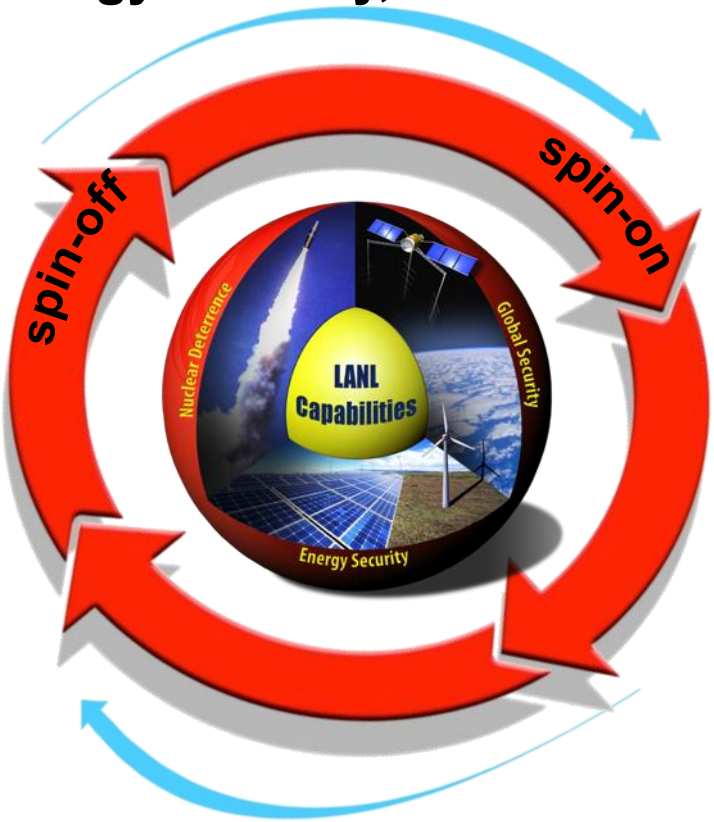
NEW MISSIONS:
Global Security, Energy Security, Economic Competitiveness…

Spin-Off Innovations

- Global Climate Modeling
- Computational Co-Design
- Robotic Telescopes
- Advanced Biofuels …

Outstanding Application to Programs

- Predicting Materials Properties
- Nuclear Forensics
- Systems Biology
- Uncertainty Quantification…



Unique Missions

- Stockpile Stewardship, Nuclear Nonproliferation

Special Blend of Capabilities and Facilities

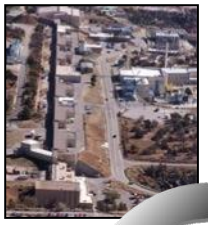
- Computational Fluid Dynamics
- Proton Radiography
- Nuclear Materials & Chemistry
- Space Sciences…

Strategic Partnerships

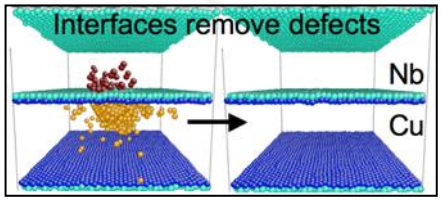
Backup Slides

Los Alamos Nurtures and Exercises very broad and deep ST&E capabilities supporting national security missions and national needs

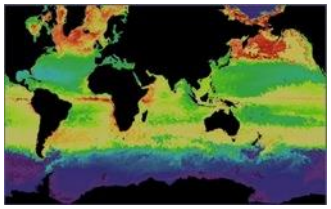
Nuclear Engineering and Technology



Accelerators & Electrodynamics

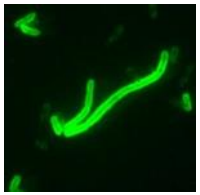


Materials

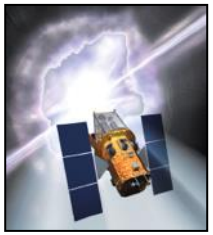


Information Science & Technology

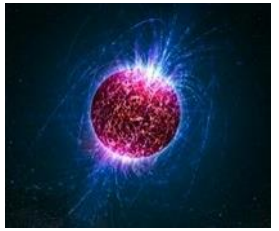
Weapons Science & Engineering



Biosciences

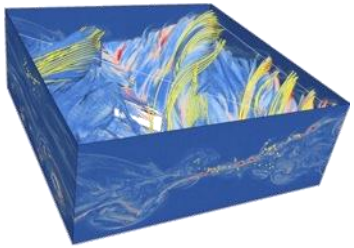


Science of Signatures

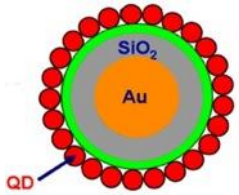


Nuclear Physics, Astrophysics & Cosmology

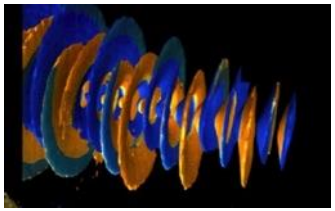
Computer & Computational Sciences



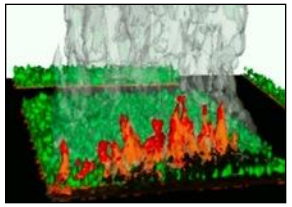
High-Energy Density Plasmas & Fluids



Chemical Science

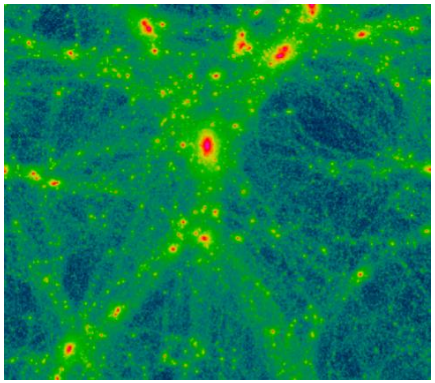


Computational Physics & Applied Mathematics



Earth & Space Sciences

“The Century of Complexity” (S. Hawking)



Cosmology: Filaments, Clusters, and Voids

Science @ Scale

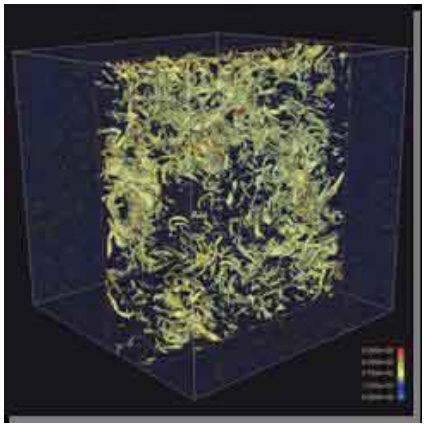
Systems of connected functional scales space, time; Emergent functions; Extreme conditions

Enabled by huge advances in Data, Simulation, Nonlinear Science…

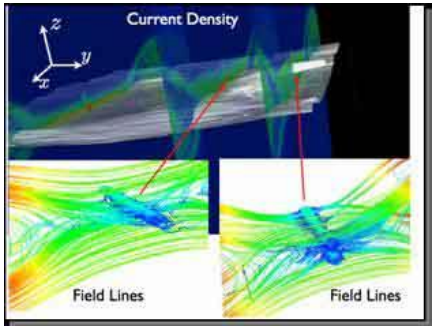
BUT….

? Origins, Measures, Consequences ?

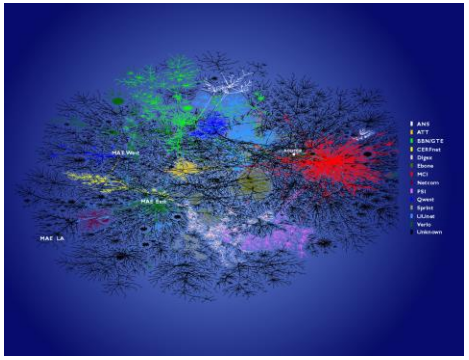
Multiscale Modeling, Simulating, Measuring ≠…at Multiple Scales: Need IS&T



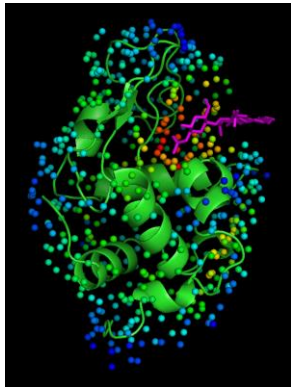
Fluid Turbulence



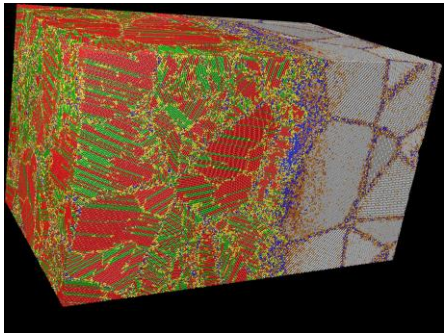
Magnetic Reconnection



Communication Networks



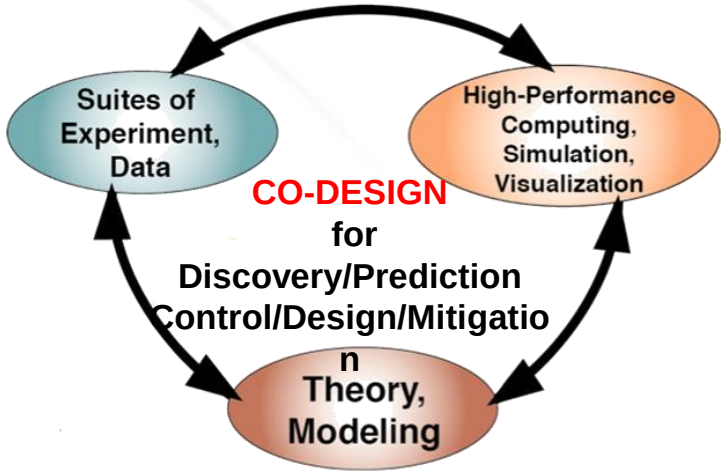
Protein Dynamics



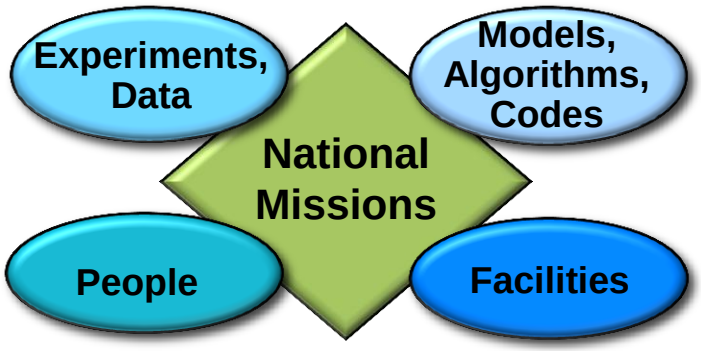
Shocked Metals

A national STE management challenge:
How we do business to impact national imperatives

- A framework of integration and collaboration for transformational ST&E at Science & Mission Frontiers
- LANL opportunities being developed: NW predictive capability framework, energy-climate, environmental, cyber, Advanced Manuf., Materials Genome … Supercomputing, MaRIE



What should next-generation facilities and campuses look like?



DOE (SC, NNSA, App. Energy) has a full spectrum of assets for the future
Integrating National Assets for Discovery, Prediction, Control, Design, Mitigation

Los Alamos' long history of moving technologies to products

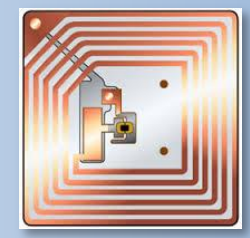
Programs

Curiosity (Rover)
ChemCam
Radioisotope Thermoelectric generator (RTG)

Hydrogen & Fuel Cells
Electrode Los Alamos Type (ELAT)
Battlefield Power

Products

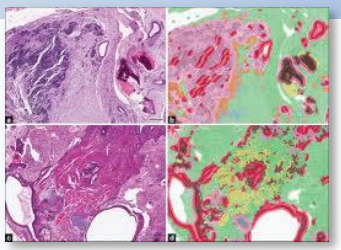
Flow Cytometry
Attune Acoustic Cytometer



Radio Frequency Identification
RFID developed for DOE, USDA, transitioned worldwide

Software

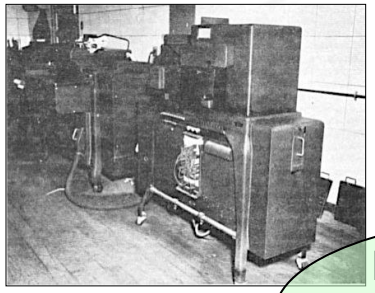
Image/Pattern Recognition
GeniePro (tumor identification)
MrSID (Geographic imaging)



Manufacturing
Reliability Technology/PowerFactoRE (manufacturing reliability
KIVA (Computational Fluid Dynamics)

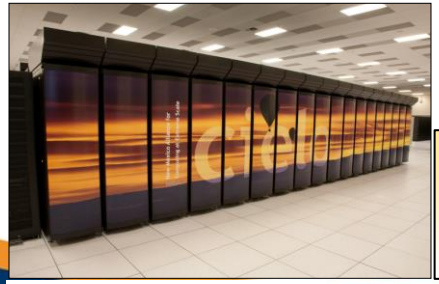
Los Alamos has been a pioneer of computing for 70 years (vector, parallel, hybrid…):

Interdisciplinary integration and mission drivers

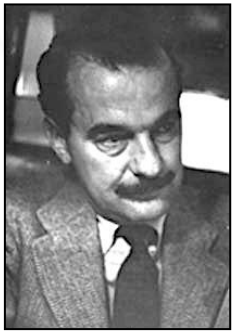


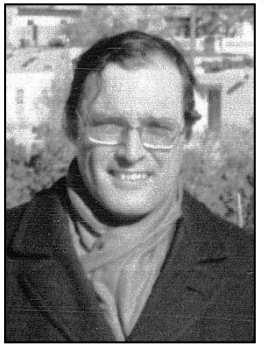
IBM 405: 1943

TMC CM-5:1992

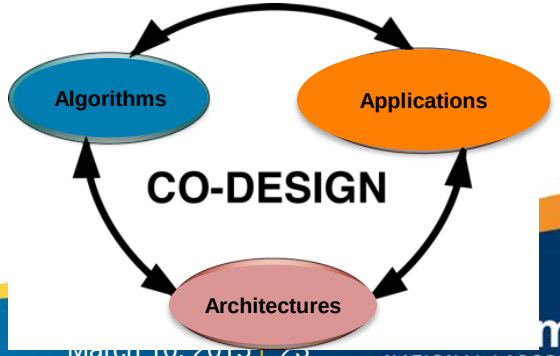


Cielo: Today, …

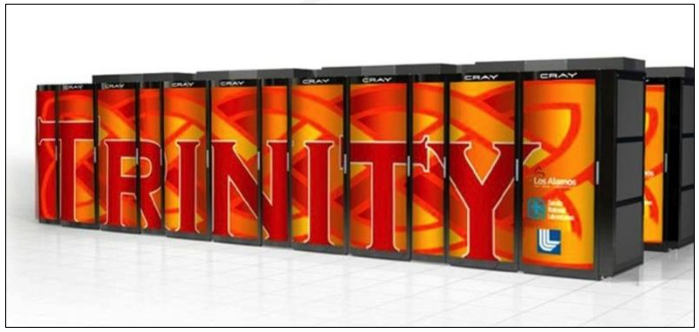




Robust Tools for Decision Makers

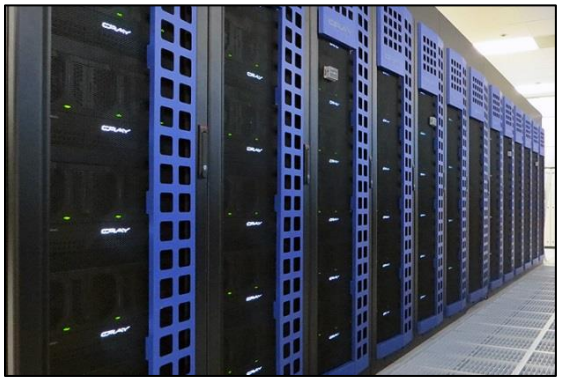


Los Alamos continues its 70-year supercomputing history



The Laboratory is a leader in providing the computing environment, systems, and technologies that support the evolution to exascale-class computing

Trinity – Cray will provide DOE-NNSA with a > 40 petaflop supercomputing system (FY16)

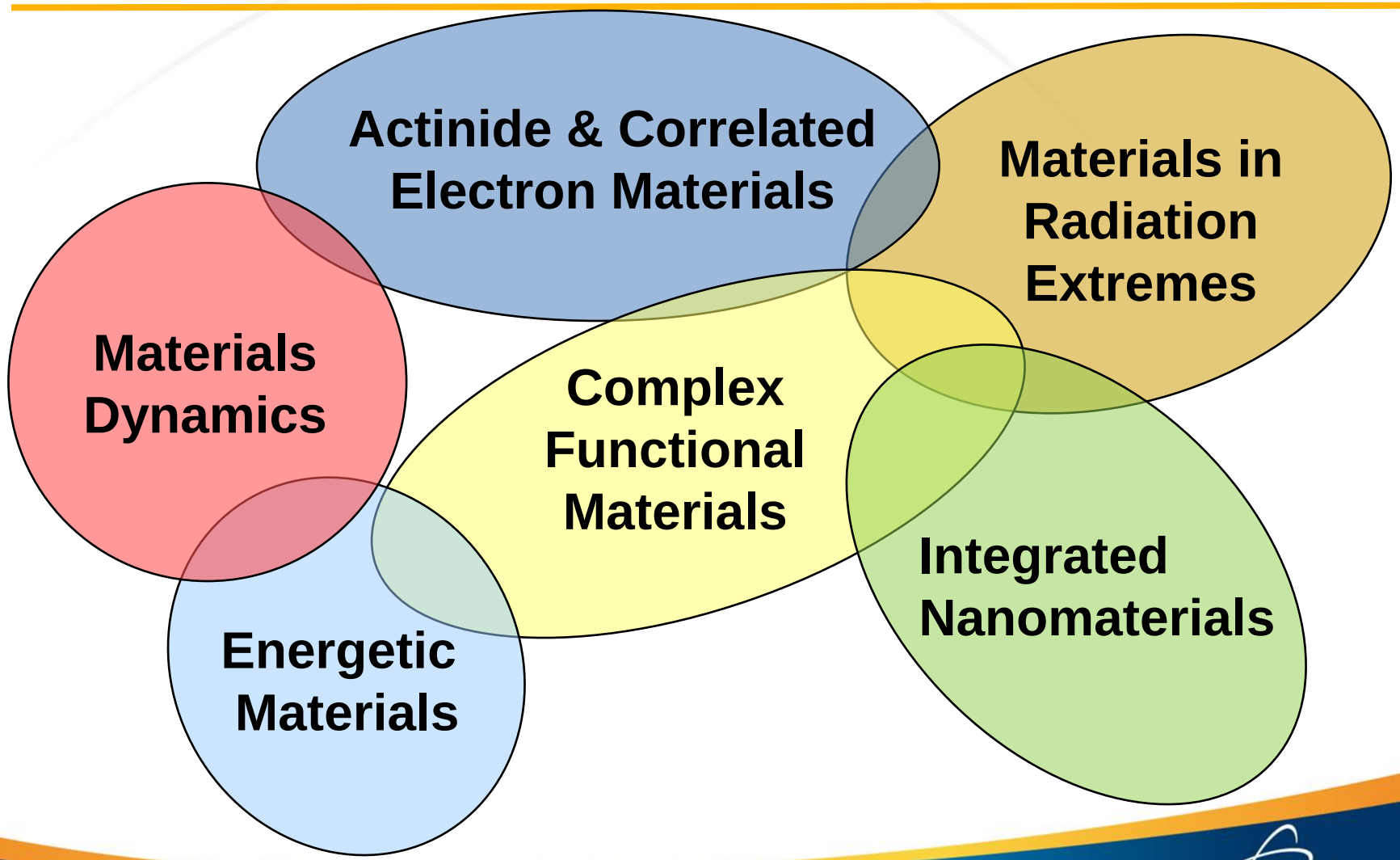


The Wolf computing system operates at 197 teraflops per second (86.3 million CPU core hours per year)

Research projects to use Wolf include materials, climate, and astrophysics

Institutional Computing provides production-computing resources for open and collaborative science at LANL

Six “Areas of Leadership” span the Materials Pillar



Embracing functional complexity in materials

Los Alamos missions have driven multi-decadal influences on Materials frontiers

Material Science History

From observing complex textures

To including lattice (& spin/charge) dynamics functionality (entropy)

Solid State Physics History

From spin/charge/lattice in idealized structures

To observing and using multiscale structure and dynamics

"1975"

Remarkable Advances

Spatio-Temporal **characterization tools** (neutrons, protons, light, spectroscopy…)

Synthesis (single crystal, films, q-dots…)

Simulations and Algorithms (MC, MD, *ab initio* QM…)

New Conceptual Frameworks

Competing Scales

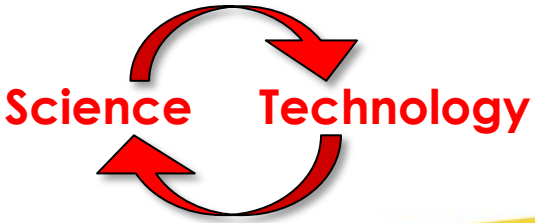
Constrained Geometry

Reduced Dimensions

Nonlinear

Non-equilibrium

• • •



Scientific Community Themes

Correlated Matter

Multiscale

Mesoscopics

Nano

• • •

Mesoscale

Materials Genome

Process-Aware Manufacturing

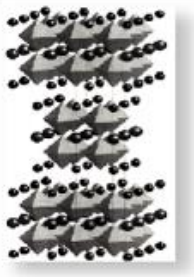
Additive Manufacturing

• • •

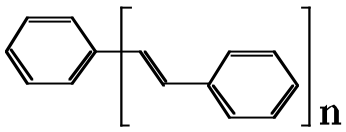
"2015"

Tuning functional multiscale complexity in "soft (electronic) matter":
Organic, inorganic, biological

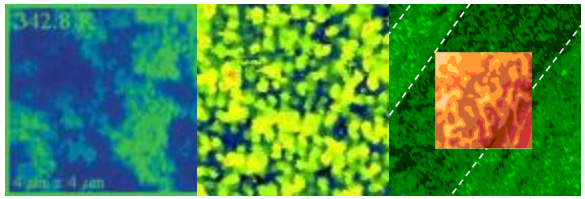
From poorly informed idealizations → ***Better "Cooking & Looking"*** → **Observing & Controlling Intrinsic Complexity**



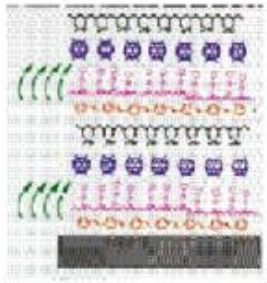
(1980)

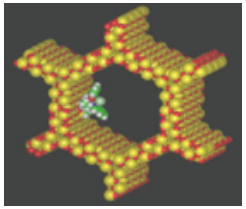


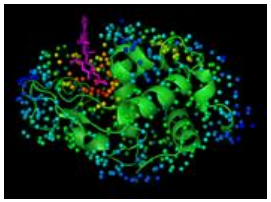
(2000)

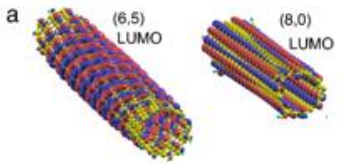


VO2 MIT (NFOM) | Gap in HighTc (STM) | CMR domains (MFM)









Coupled
Spin-Charge-Lattice;
Short-Long Competition;
Geometric Frustration

Strongly correlated,
intrinsically
soft, multiscale, glassy;

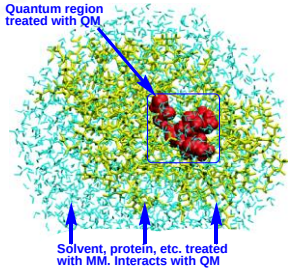
Aging, Healing, Learning

Systems/Networks
of connected,
functional scales
(structural and
electronic/magnetic/optical)

NEED: Tools to probe complexity and a framework for understanding/controlling responses and applications
(cf. US DOE-BES "Mesoscale Initiative")

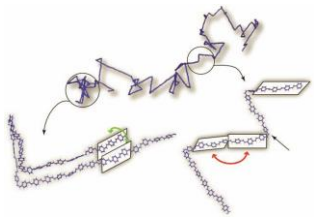
Remarkable emerging capabilities:
Spatio-temporal scales

THEORY/SIMULATION



Quantum Mechanics/ Molecular Mechanics (QM/MM) modeling

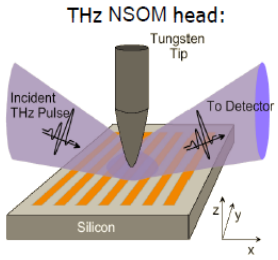
- Treats large segments of material
- Realistic dielectric environment

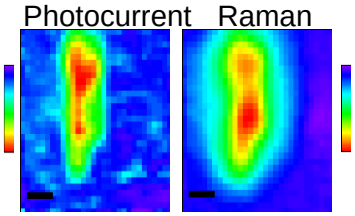


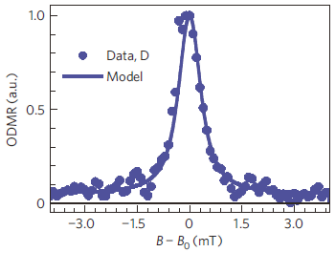
Advanced transport models

- Use parameters derived from the electronic structure calculations
- Fully multiscale modeling

EXPERIMENT







THz Near-Field Scanning Optical Microscope (THz - NSOM)

- Under 100-nm spatial resolution (i.e., local conductivity)
- Probe charge dynamics on <1-ps time scales

Optical NSOM/ Atomic Force Microscope (AFM)

- Correlate optical response (Raman, PL, TRPL) and morphology with <50-nm spatial resolution

Simultaneous Optical-Electrical Characterization Capability

- Correlate optical responses with charge separation/photocurrent generation efficiencies
- Probe existence of interfacial CTC states

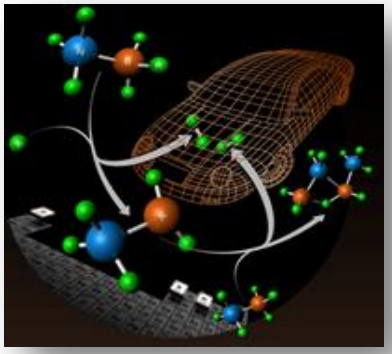
Optically Detected Magnetic Resonance (ODMR) spectroscopy

- Direct measurement of the spatial wave function extent of charges (polarons)
- Detailed information on the various spin states (e.g., triplets)
- Useful tool for many spintronics investigations

Los Alamos' Energy Security Plan identifies areas of strategic focus and DOE alignment

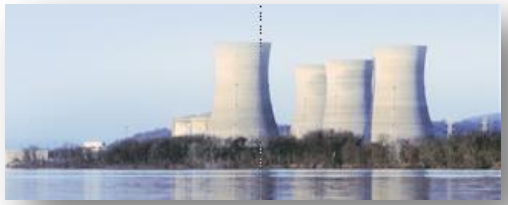
★Materials and Concepts for Clean Energy

- Enabling new sources of energy and more efficient utilization
- Generating novel technologies for the production and use of fossil energy



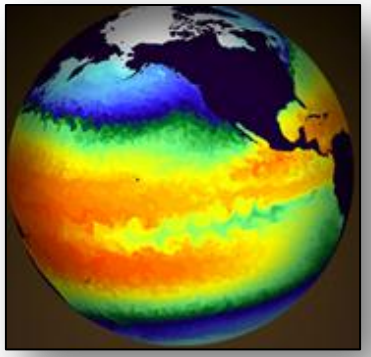
★Sustainable Nuclear Energy

- Understanding the lifetime of fuels and components, safety options, disposal of waste and long-term storage, and remediation of environmental impact
- Creating advanced technology for existing reactors and new concepts in nuclear power generation



★Mitigating Impacts of Global Energy Demand Growth

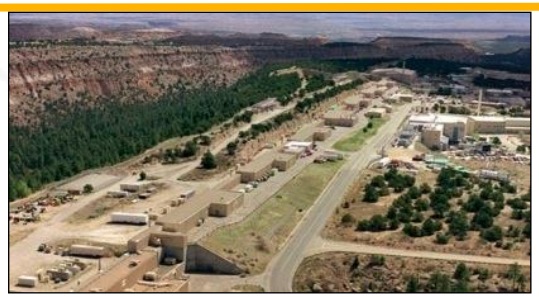
- Developing predictive tools for climate, earth, and water systems, including their impacts on communities and infrastructure
- Creating and deploying measurement systems, and integrating data at all length scales to verify models and inform decisions



LANL has many unique facilities

Metropolis Center for Modeling & Simulation

High Explosive Laboratories



Los Alamos Neutron Science Center

Chemistry and Metallurgy Building

Dual Axis Radiographic Hydrotest Facility

Plutonium Processing Facility

Chemistry & Metallurgy Research Replacement (RLUOB)

SIGMA Building

…and many more!